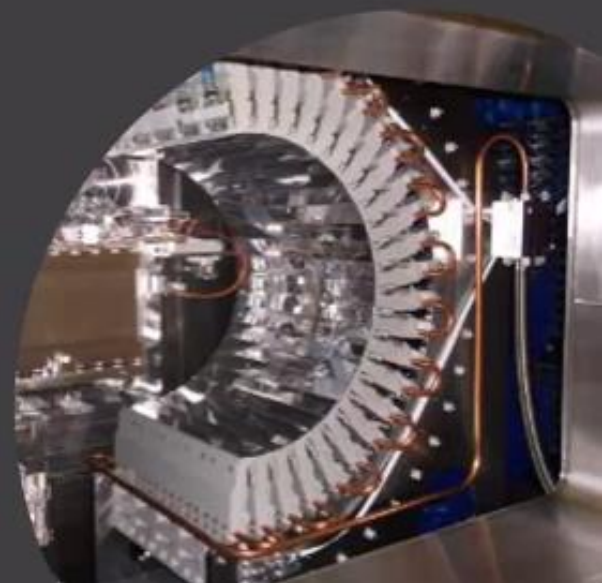


December 2021

Diamond MX operation updates

dls.mx



MX Team



Group Support

Felicity Bertram
Marco Mazzorana
Elliot Nelson

Industry

Alex Dias
Christofer Bjorkelid
Ailsa Powell
Jitka Waterman

Software



Controls



Technicians



Engineers



Dave Hall – MX Group Leader

What are we offering



Unattended automated data collection



Remote access, on-site and mail-in (Industry) to I03, I04, I04-1, I24 and VMXi



Mail-in access to long wavelength beamline I23

See Armin Wagner talk



XChem on I04-1

See Daren Fearon talk



Serial Synchrotron Crystallography on I24

See Robin Owen talk



XFEL Hub

Continuing to support UK community with access to FELs

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Access at Diamond MX



Responsive Mode Access

Schedule based on samples delivered to site.
6 days median turnaround from delivery to site.



Regular scheduling

Pre-book slots in conjunction with PBS and mx-usersupport and ship samples in for these or come to site



Access continues for existing proposals till 4th March 22 Users who had time awarded in allocation period 30 (Jul - Dec 2021)



Continue to prioritise COVID-19 projects

Via rapid access call



New users

Submit rapid access application at uas.diamond.ac.uk

Automated Unattended Data Collection Status



Since opening up to community on I03 following Covid-19 lockdown June 2020:



>50 groups – Academic and Industrial



>1,000 visits



60,000 samples - 9,400 in last four weeks alone as now running across beamlines



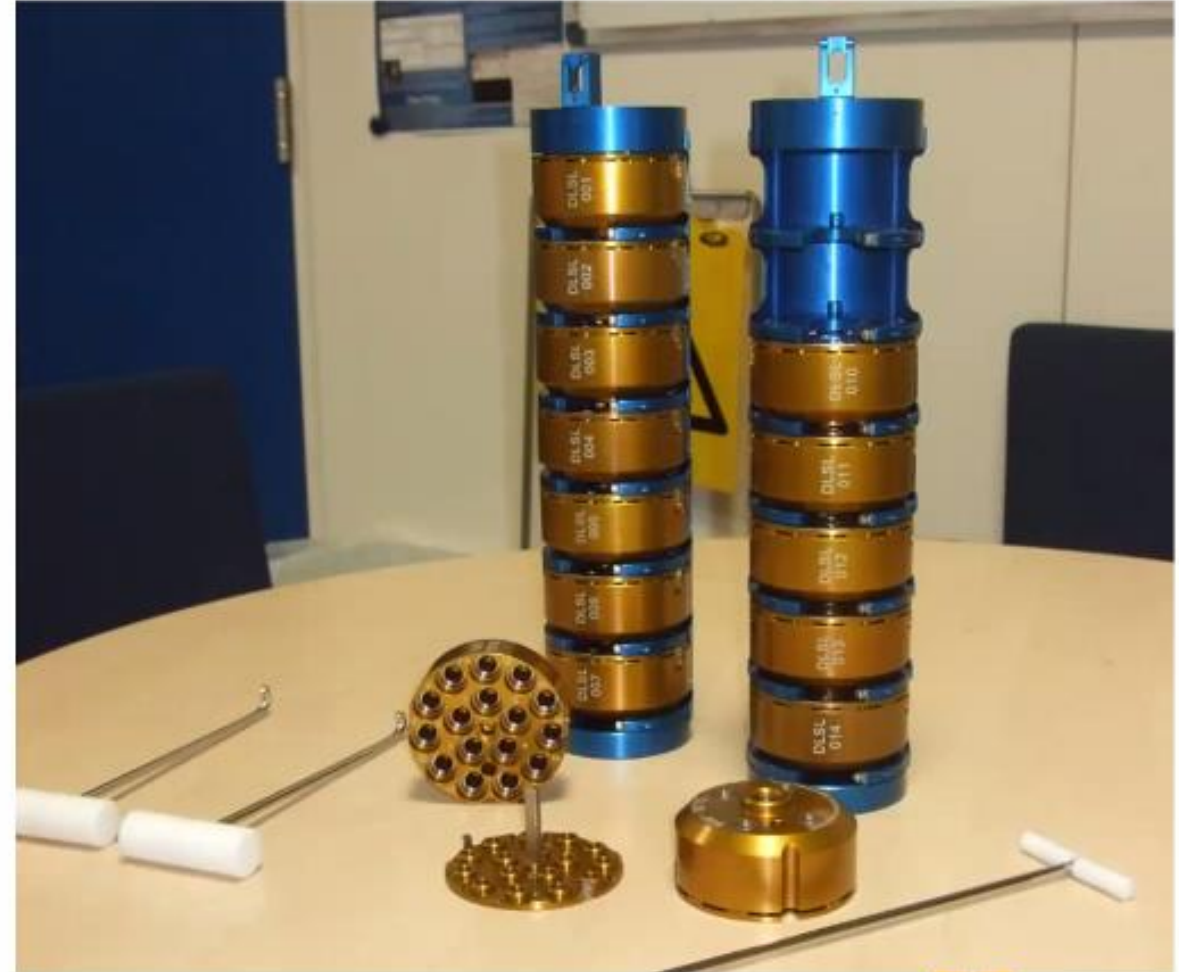
Median turn around time from arrival to collection is 3.5 days



If you've not tried it already give it a whirl – see dls.mx/UDC for details

Some practicalities

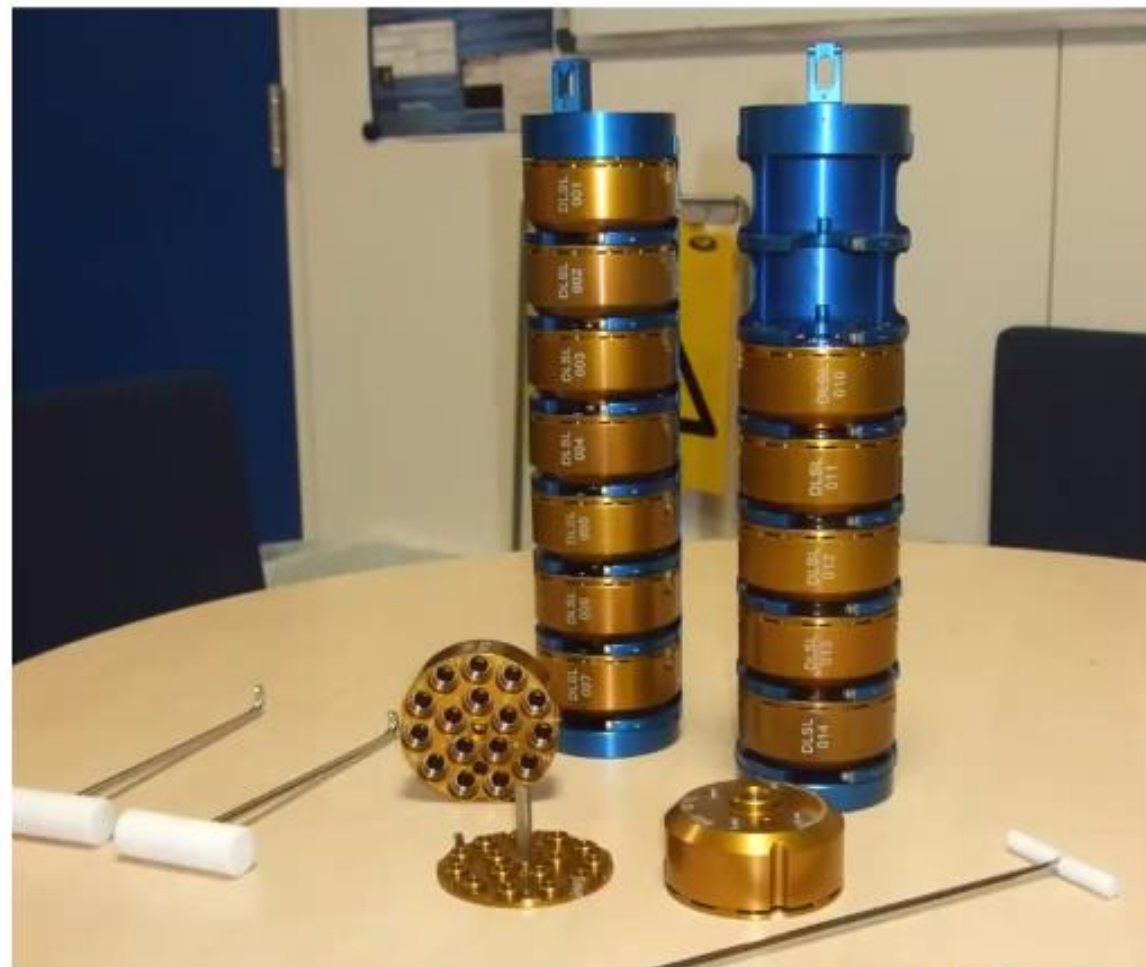
- Responsive mode access provides flexibility for you and us to respond to changing circumstances
- It has changed the workload at Diamond and we would appreciate your support with some simple guidelines
- Shipping and sample management
 - We have added the ERA Admin role in UAS so you can delegate workload
 - Please define your pucks before shipping (safety and helps us with scheduling on beamlines)
 - Please carry out regular maintenance checks on your Dewars, Pucks and Pins
 - We request you use shelved puck holders
 - For Non UK users – dynamic circumstances with shipping following BREXIT continue to present challenges

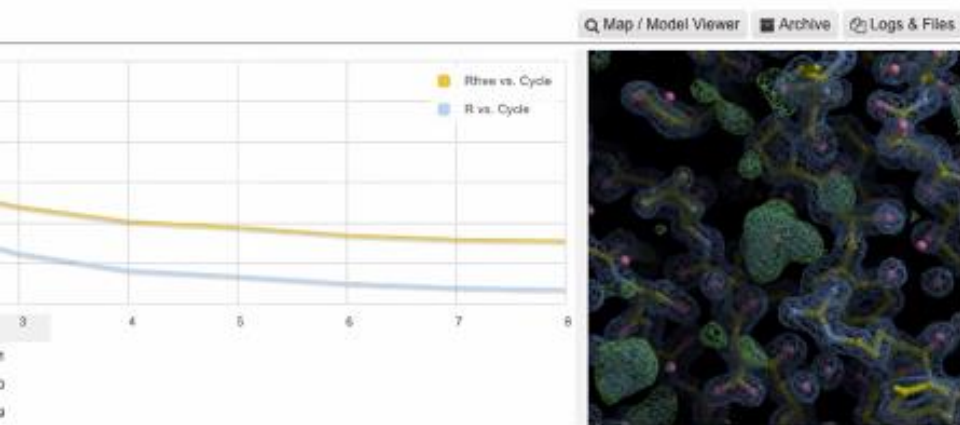
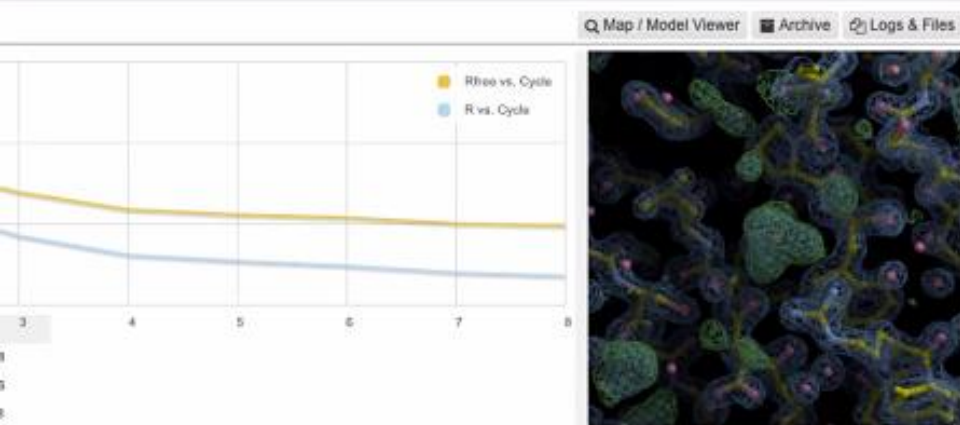


Some practicalities

- Please be reasonable in your availability particularly over weekends
 - Can greatly delay you getting timely beamtime, makes scheduling and management more complicated and slows down the return of your Dewars, pucks and pins
- To help you monitor usage BAG PI/ACs will receive regular email updates on usage
 - We are working on an automated system to report UDC usage
- Talk to us!
 - Contact PBS, your local contact and/or mx-usersupport@diamond.ac.uk

**We are more optimised than ever before so
continue to send samples
(in the New Year!)**





Using AI models in MX pipelines – dls.mx/alphafold

- Two pipelines for molecular replacement exist using either sequence or PDB file added to a “Protein” in ISPyB
 - DIMPLE – runs on all data reduction pipelines (fast_dp, xia2 3dii and xia2 dials + multiplex runs). If poor Rfactor returned for diff map then deploys Phaser for MR attempt
 - MrBUMP – runs on all data reduction pipelines except for fast_dp and uses both PDB models and sequences
- Alphafold now deployed in Diamond pipelines**
 - Add a sequence in ISPyB to trigger Alphafold
 - Pruned output from this inserted into ISPyB for use against our automated MR pipelines
- Please provide feedback on both successes and failures

Current Vacancies



- I24 PDRA
- MX beamline scientist (Diamond-II support)
- <https://www.diamond.ac.uk/Careers/Vacancies.html>
- Summer placements 2022
 - <https://www.diamond.ac.uk/Careers/Students/Summer-Placement/2022-Summer-Placements1.html>

Thank you

Beam is back on 19th January – see you in the New Year!